

Optimizing the Gutman index: A study of minimum values under transformations of graphs

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Abstract: The extremal Gutman index is a concept in graph theory that studies the maximum or minimum value of the Gutman index for a particular class of graphs. This research area is concerned with finding the graphs that have the lowest possible Gutman index within a set of graphs that have been transformed in some way, such as by adding or removing edges or vertices. The study of the extremal Gutman index can provide insights into the structure and stability of graphs, and has applications in a range of fields, including chemical graph theory and social network analysis. By understanding the graphs that have the lowest possible Gutman index, researchers can better understand the fundamental principles of graph stability and the role that different graph transformations play in affecting the overall stability of a graph. The research in this area is ongoing and continues to expand as new techniques and algorithms are developed. The findings from this research have the potential to have a significant impact on a wide range of fields and can lead to new and more effective ways of analyzing and understanding complex systems and relationships in a variety of applications. This paper focuses on the study of specific types of trees that are defined by fixed parameters and characterized based on their Gutman index. Specifically, we explore the structural properties of graphs that have the lowest Gutman index within these classes of trees. To achieve this, we utilize various graph transformations that either decrease or increase the Gutman index. By applying these transformations, we construct trees that satisfy the desired criteria.

Keywords: Gutman index, transformation; diameter, balance spider, extremal trees, matching number, domination number.

AMS Subject classification: 05C09, 05C92, 05C90

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1. Introduction

The Gutman index is a mathematical concept used in graph theory to measure the overall "stability" of a graph, also known as a measure of graph harmonicity. It was introduced by a mathematician I. Gutman in the 1970s. The Gutman index can be useful in various applications, such as in chemical graph theory, where it is used to analyze the stability of chemical compounds, and in the study of social networks, where it can be used to quantify the balance and structure of relationships between individuals in a network. It is important to note that the Gutman index is just one of many measures of stability in graph theory, and its suitability for a given application depends on the specific requirements and objectives of the analysis.

One area of research in the Gutman index focuses on the computational aspects of its calculation. Researchers have developed efficient algorithms for computing the Gutman index, including both exact and approximation algorithms. These algorithms have been implemented and tested on a variety of graphs, including large-scale networks. Another area of research explores the relationship between the Gutman index and other graph-theoretic concepts, such as distance-based indices, degree-based indices, and Wiener index. Researchers have shown that the Gutman index is closely related to these indices, and have established mathematical connections between them. Finally, there has been a growing interest in the study of the extremal values of the Gutman index for specific classes of graphs. Researchers have investigated the conditions under which graphs have maximum or minimum values of the Gutman index, and have developed techniques for constructing graphs with optimal values of the Gutman index. Overall, the literature on the Gutman index is extensive and covers a wide range of topics, demonstrating the versatility and importance of this concept in graph theory. The following is a brief literature review of some of the key works in this area.

When Harry Wiener created the Wiener index in 1947, the history of topological descriptors officially started. The study of many mathematical features of graphs has made topological indices a popular subject. They are used widely in chemistry, biology, and many other disciplines [6–9]. The oldest index with well-studied mathematical and chemical applications is the Wiener index. In order to clarify the relationships between the molecular structures [25] of paraffin and their boiling points, Wiener devised the Wiener index, which is typically translated as:

$$W(H) = \sum_{h_1, h_2 \subseteq V(H)} d_H(h_1, h_2),$$

where $d_H(h_1, h_2)$ is the distance between h_1 and h_2 .

The Gutman index (*Gut*) is a natural extension of the Wiener index. The Gutman index of a finite connected graph H is defined as

$$Gut(H) = \sum_{h_1, h_2 \subseteq V(H)} (\deg_H h_1 d_H h_2) d_H(h_1, h_2),$$

For increasing trees, the Gutman index was investigated by Kazemi and Meimeondari [16]. Gutman [12] introduces the concept of degree-based topological indices, which include the Gutman index as a special case. It defines the Gutman index and establishes its basic properties. In [24], Réti et al. investigates the bond-additive and atoms-pair-additive indices of graphs. In [1], authors investigate the reverse-degree-based topological indices of fullerene cage networks. In [17] the authors studied the topological invariants of nanocones and fullerenes.

In [1], authors investigate the reverse-degree-based topological indices of fullerene cage networks. In [17] the authors studied the topological invariants of nanocones and fullerenes. Raza and Ali [23], presented bounds on the Zagreb indices for molecular (n, m) graphs along with the identification of the graphs attaining them. Arockiaraj et al. [5] utilized the vertex cut method to compute some indices for silicate networks. Li and Zhang [20] investigated the mathematical properties of the multiplicative weighted Harary index using various transformations. Hua [15] employed transformations to study the extreme characteristics of the Wiener index and the molecular topological index. Li and Meng [18] and He et al. [14] examined the behavior of the some indices of graphs obtained by edge operations. For further mathematical studies, refer to [2, 3, 10, 11, 19, 21, 22, 26, 27].

An independent edge set of a subset of $E(H)$ is defined as a set where no two edges share the same H vertex. The maximum independent edge set is the largest set among all independent edge sets. The matching number, denoted by $\nu(H)$, is the total number of matches possible for H . A dominating set for H is a subset of $V(H)$ such that every vertex not in the subset is connected to at least one of its members. The vertices in the dominating set are called dominating vertices. The minimum number of dominating sets for H is referred to as the domination number, which is abbreviated as $\omega(H)$. This paper focuses on the study of specific types of trees that are defined by fixed parameters and characterized based on their Gutman index. Specifically, we explore the structural properties of graphs that have the lowest Gutman index within these classes of trees. To achieve this, we utilize various graph transformations that either decrease or increase the Gutman index. By applying these transformations, we construct trees that satisfy the desired criteria.

2. Graph transformations and their effects on the Gutman index

Graph transformations are a powerful tool in graph theory for modifying the structure of a graph in order to better understand its properties [18]. When applied to the Gutman index, these transformations can have a significant impact on its value. The study of graph transformations and their effects on the Gutman index is an active area of research, with the goal of finding the conditions under which these transformations result in graphs with optimal values of the Gutman index. This line of research has important applications in various fields, including chemistry, where the stability of chemical compounds can be analyzed using the Gutman index, and network analysis,

where the stability of social networks can be evaluated. By investigating the effects of graph transformations on the Gutman index, researchers can gain insight into the structural properties of graphs that are critical for stability and harmonicity.

2.1. α -transformation

The α -transformation is defined as follows: Consider two nontrivial trees Γ_1 and Γ_2 . Let $x \in V(\Gamma_1)$ and $y \in V(\Gamma_2)$, and connect Γ_1 to Γ_2 with a path $P_k = a_1, a_2, a_3, \dots, a_k$ by identifying x with a_1 and y with a_k . The resulting graph is denoted by \mathbb{G} . The graphs obtained from \mathbb{G} by moving Γ_2 from a_k to a_1 are denoted by \mathbb{G}' . The operation of obtaining \mathbb{G}' from the original graph \mathbb{G} is called the α -transformation.

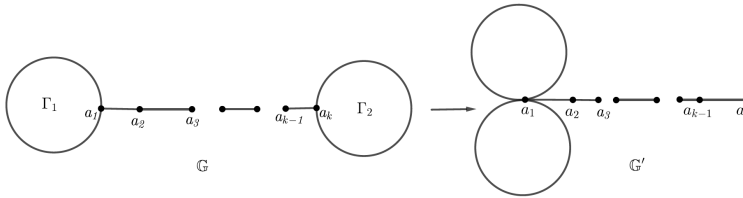


Figure 1. α -transformation

Theorem 1. Let \mathbb{G}' be a connected graph with $n \geq 2$ vertices obtained from \mathbb{G} by α -transformation (see Figure 1). Then $Gut(\mathbb{G}) > Gut(\mathbb{G}')$.

Proof. Let us denote $\mathbb{B} = V(\Gamma_1) \cup V(\Gamma_2) \cup P_k \setminus \{a_1, a_k\}$. Then

$$\begin{aligned}
 Gut(\mathbb{G}) - Gut(\mathbb{G}') &= \sum_{\substack{p \in \{a_1, a_k\} \\ v \in \mathbb{B}}} (d_{\mathbb{G}}(p).d_{\mathbb{G}}(v))d_{\mathbb{G}}(p, v) - \sum_{\substack{p \in \{a_1, a_k\} \\ v \in \mathbb{B}}} (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(v))d_{\mathbb{G}'}(p, v) \\
 &+ \sum_{\substack{p \in V(\Gamma_1) \setminus \{a_1\} \\ q \in V(\Gamma_2) \setminus \{a_k\}}} (d_{\mathbb{G}}(p).d_{\mathbb{G}}(q))d_{\mathbb{G}}(p, q) - \sum_{\substack{p \in V(\Gamma_1) \setminus \{a_1\} \\ q \in V(\Gamma_2) \setminus \{a_k\}}} (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(q))d_{\mathbb{G}'}(p, q) \\
 &+ \sum_{\substack{p \in V(\Gamma_1) \cup V(\Gamma_2) \setminus \{a_1, a_k\} \\ q \in V(P_k) \setminus \{a_1, a_k\}}} (d_{\mathbb{G}}(p).d_{\mathbb{G}}(q))d_{\mathbb{G}}(p, q) \\
 &- \sum_{\substack{p \in V(\Gamma_1) \cup V(\Gamma_2) \setminus \{a_1, a_k\} \\ q \in V(P_k) \setminus \{a_1, a_k\}}} (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(q))d_{\mathbb{G}'}(p, q) \\
 &+ \sum_{p, q \in V(\Gamma_1) \setminus \{a_1\}} (d_{\mathbb{G}}(p).d_{\mathbb{G}}(q))d_{\mathbb{G}}(p, q) - \sum_{p, q \in V(\Gamma_1) \setminus \{a_1\}} (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(q))d_{\mathbb{G}'}(p, q) \\
 &+ (d_{\mathbb{G}}(a_1).d_{\mathbb{G}}(a_k))d_{\mathbb{G}}(a_1, a_k) - (d_{\mathbb{G}'}(a_1).d_{\mathbb{G}'}(a_k))d_{\mathbb{G}'}(a_1, a_k).
 \end{aligned}$$

It is easy to see from Figure 1 that for $p \in V(\Gamma_1) \setminus \{a_1\}$ (respectively $V(\Gamma_2) \setminus \{a_k\}, V(P_k) \setminus \{a_1, a_k\}$), we have $d_{\mathbb{G}}(p) = d_{\mathbb{G}'}(p)$. If $p \in V(\Gamma_1) \setminus \{a_1\}$, then $d_{\mathbb{G}'}(p, a_i) = d_{\mathbb{G}}(p, a_i)$ for all $i = 1, 2, \dots, k - 1$ and if $p \in V(\Gamma_2) \setminus \{a_k\}$, then $d_{\mathbb{G}'}(p, a_i) = d_{\mathbb{G}}(p, a_{k-i+1})$ for all $i = 1, 2, \dots, k - 1$. So, we have

$$\sum_{p, q \in V(\Gamma_1) \setminus \{a_1\}} [(d_{\mathbb{G}}(p).d_{\mathbb{G}}(q))d_{\mathbb{G}}(p, q) - (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(q))d_{\mathbb{G}'}(p, q)] = 0.$$

Also, we have

$$\sum_{\substack{p \in V(\Gamma_1) \cup V(\Gamma_2) \setminus \{a_1, a_k\} \\ q \in V(P_k) \setminus \{a_1, a_k\}}} [(d_{\mathbb{G}}(p).d_{\mathbb{G}}(q))d_{\mathbb{G}}(p, q) - (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(q))d_{\mathbb{G}'}(p, q)] = 0$$

Thus, we have only the following expressions:

$$\begin{aligned} \sum_1 &= \sum_{\substack{p \in \{a_1, a_k\} \\ q \in \mathbb{B}}} (d_{\mathbb{G}}(p).d_{\mathbb{G}}(q))d_{\mathbb{G}}(p, q) - \sum_{\substack{p \in \{a_1, a_k\} \\ q \in \mathbb{B}}} (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(q))d_{\mathbb{G}'}(p, q) \\ \sum_2 &= \sum_{\substack{p \in V(\Gamma_1) \setminus \{a_1\} \\ q \in V(\Gamma_2) \setminus \{a_k\}}} (d_{\mathbb{G}}(p).d_{\mathbb{G}}(q))d_{\mathbb{G}}(p, q) - \sum_{\substack{p \in V(\Gamma_1) \setminus \{a_1\} \\ q \in V(\Gamma_2) \setminus \{a_k\}}} (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(q))d_{\mathbb{G}'}(p, q) \\ \sum_3 &= (d_{\mathbb{G}}(a_1).d_{\mathbb{G}}(a_k))d_{\mathbb{G}}(a_1, a_k) - (d_{\mathbb{G}'}(a_1).d_{\mathbb{G}'}(a_k))d_{\mathbb{G}'}(a_1, a_k). \end{aligned}$$

Thus, we have

$$Gut(\mathbb{G}) - Gut(\mathbb{G}') = \sum_1 + \sum_2 + \sum_3.$$

So, we need to show that $\sum_1 + \sum_2 + \sum_3 > 0$. To show this let $d_{\Gamma_1}(a_1) = m_1$ and $d_{\Gamma_2}(a_k) = m_2$. It is easy to see that $d_{\mathbb{G}}(a_1, a_i) = d_{\mathbb{G}'}(a_k, a_{k-i+1})$, for all $i = 1, 2, \dots, k - 1$. Thus

$$\sum_1 = \sum_1^1 + \sum_1^2 + \sum_1^3 + \sum_1^4 + \sum_1^5,$$

where

$$\begin{aligned} \sum_1^1 &= \sum_{i=2}^{k-1} 2(m_1 + 1)d_{\mathbb{G}}(a_1, a_i) + \sum_{i=2}^{k-1} 2(m_2 + 1)d_{\mathbb{G}}(a_k, a_i) - \sum_{i=2}^{k-1} 2(m_1 + m_2 + 1)d_{\mathbb{G}'}(a_1, a_i) \\ &\quad - \sum_{i=2}^{k-1} (2)d_{\mathbb{G}'}(a_k, a_i). \end{aligned}$$

Since $d_{\mathbb{G}}(a_1, a_i) = d_{\mathbb{G}'}(a_k, a_{k-i+1})$, so $\sum_1^1 = 0$. Now

$$\begin{aligned} \sum_1^2 &= \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} (d_{\mathbb{G}}(p).d_{\mathbb{G}}(a_1))d_{\mathbb{G}}(p, a_1) - \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} (d_{\mathbb{G}'}(p).d_{\mathbb{G}'}(a_1))d_{\mathbb{G}'}(p, a_1) \\ &= \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} [(m_1 + 1)d_{\mathbb{G}}(p) - (m_1 + m_2 + 1)d_{\mathbb{G}}(p)]d_{\mathbb{G}}(p, a_1) \\ &= \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} (-m_2)d_{\mathbb{G}}(p)d_{\mathbb{G}}(p, a_1). \end{aligned}$$

Similarly, we have

$$\begin{aligned} \sum_1^3 &= \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} (d_G(p).d_G(a_k))d_G(p, a_k) - \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} (d_{G'}(p).d_{G'}(a_k))d_{G'}(p, a_k) \\ &= \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} [(m_2 + 1)d_G(p) - (1)d_G(p)]d_G(p, a_k). \end{aligned}$$

As $d_G(p, a_k) = d_G(p, a_1) + k - 1$, so

$$\sum_1^3 = \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} (m_2)d_G(p)[d_G(p, a_1) + k - 1].$$

Hence

$$\sum_1^2 + \sum_1^3 = m_2(k - 1) \sum_{p \in V(\Gamma_1) \setminus \{a_1\}} d_G(p).$$

By similar argument, we have

$$\begin{aligned} \sum_1^4 &= \sum_{w \in V(\Gamma_2) \setminus \{a_k\}} (d_G(w).d_G(a_1))d_G(w, a_1) - \sum_{w \in V(\Gamma_2) \setminus \{a_k\}} (d_{G'}(w).d_{G'}(a_1))d_{G'}(w, a_1) \\ \sum_1^5 &= \sum_{w \in V(\Gamma_2) \setminus \{a_k\}} (d_G(w).d_G(a_k))d_G(w, a_k) - \sum_{w \in V(\Gamma_2) \setminus \{a_k\}} (d_{G'}(w).d_{G'}(a_k))d_{G'}(w, a_k). \end{aligned}$$

But $d_{G'}(w, a_1) = d_G(w, a_k)$ and $d_{G'}(w, a_k) = d_G(w, a_k) + k - 1$, for all $w \in V(\Gamma_2) \setminus \{a_k\}$, so, we have

$$\sum_1^4 + \sum_1^5 = m_1(k - 1) \sum_{w \in V(\Gamma_2) \setminus \{a_k\}} d_G(w).$$

Denote $\sum_{w \in V(\Gamma_2) \setminus \{a_k\}} d_G(w) = \beta > 0$ and $\sum_{p \in V(\Gamma_1) \setminus \{a_1\}} d_G(p) = \alpha > 0$, then

$$\sum_1 = \sum_1^1 + \sum_1^2 + \sum_1^3 + \sum_1^4 + \sum_1^5 = (k - 1)[m_2\alpha + m_1\beta] > 0,$$

since $k > 1$.

Now

$$\sum_2 = \sum_{\substack{p \in V(\Gamma_1) \setminus \{a_1\} \\ q \in V(\Gamma_2) \setminus \{a_k\}}} (d_G(p).d_G(q))d_G(p, q) - \sum_{\substack{p \in V(\Gamma_1) \setminus \{a_1\} \\ q \in V(\Gamma_2) \setminus \{a_k\}}} (d_{G'}(p).d_{G'}(q))d_{G'}(p, q),$$

$d_{G'}(p, q) = d_G(p, q) - k + 1$ for all $p \in V(\Gamma_1) \setminus \{a_1\}$ and $q \in V(\Gamma_2) \setminus \{a_k\}$. Thus

$$\sum_2 = (k - 1) \sum_{\substack{p \in V(\Gamma_1) \setminus \{a_1\} \\ q \in V(\Gamma_2) \setminus \{a_k\}}} (d_G(p).d_G(q)) = (k - 1)\alpha\beta > 0,$$

since $k > 1$. It is easy to see that $\sum_3 = m_1m_2(k - 1) > 0$, which complete the proof. □

2.2. β -transformation

To define β -transformation, consider a nontrivial tree Γ such that $V(\Gamma) = n$ and $E(\Gamma) = n - 1$. Let us take $ab \in E(\Gamma)$ such that $d_\Gamma(a) = q + 1 (q \geq 2)$, $d_\Gamma(b) = t$ and subtrees $\Gamma_1, \Gamma_2, \dots, \Gamma_q$ with root vertices $c_1, c_2, c_3, \dots, c_q$ connected to the vertex b of the tree Γ . Furthermore, $v\Gamma_q \cong P_l$ and a subgraph \mathbb{G}_1 having b must contains a path $P_k = b_1, b_2, \dots, b_k$ with $k \geq l$ and b_1 is attached to the vertex b with $|V(\mathbb{G}_1)| = l + 2$. Now the graph Γ' obtained form Γ as $\Gamma' = \Gamma - \{ac_i \mid 1 \leq i \leq q - 1\} + \{bc_i \mid 1 \leq i \leq q - 1\}$. To obtained Γ' from the original tree Γ is called β transformation as shown in the Figure 2.2.

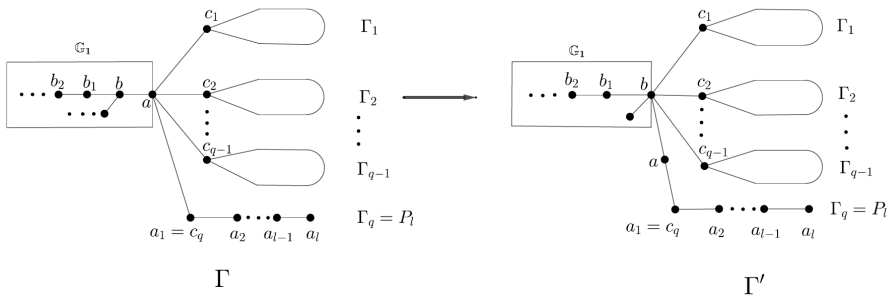


Figure 2. β -transformation

Theorem 2. Let Γ' be a connected tree with $n \geq 2$ vertices obtained from Γ by β -transformation (see Figure 2.2). Then

$$Gut(\Gamma) > Gut(\Gamma').$$

Proof. Let us denoted the graph $\mathbb{G} = \bigcup_{i=1}^{q-1} \Gamma_i$ and $\Gamma_q \cong P_l = a_1, a_2, \dots, a_l$ with $a_1 = c_m$. From Figure 2.2, it is easy to note that for $x, y \in V(\mathbb{G}_1) \setminus \{b\}$ (respectively $V(\mathbb{G}_1)$ and $V(P_l)$ for all $d_\Gamma(x) = d_{\Gamma'}(x)$ and $d_\Gamma(x, y) = d_{\Gamma'}(x, y)$. Then, we have

$$Gut(\mathbb{G}) - Gut(\mathbb{G}') = \sum_1 + \sum_2 + \sum_3,$$

where

$$\begin{aligned} \sum_1 &= \sum_{\substack{x \in \{a,b\} \\ y \in V(\Gamma) \setminus \{a,b\}}} [(d_\Gamma(x).d_\Gamma(y))d_\Gamma(x, y) - (d_{\Gamma'}(x).d_{\Gamma'}(y))d_{\Gamma'}(x, y)] \\ \sum_2 &= (d_\Gamma(a).d_\Gamma(b))d_\Gamma(a, b) - (d_{\Gamma'}(a).d_{\Gamma'}(b))d_{\Gamma'}(a, b) \\ \sum_3 &= \sum_{\substack{x \in V(\mathbb{G}_1) \cup V(P_l) \setminus \{b\} \\ y \in V(\mathbb{G})}} [(d_\Gamma(x).d_\Gamma(y))d_\Gamma(x, y) - (d_{\Gamma'}(x).d_{\Gamma'}(y))d_{\Gamma'}(x, y)]. \end{aligned}$$

Now, we prove that $\sum_1 + \sum_2 + \sum_3$ is positive. Since the length of the path P_k is greater or equal than the length of the path P_l , so $k \geq l$ and $\deg(b_i) \geq 2$ for all $i = 1, 2, \dots, k - 1$.

Since $\Gamma = \mathbb{G}_1 \setminus \{P_k\} \cup \mathbb{G} \cup P_k \cup P_l$, hence \sum_1 can be further written as four sums as below:

$$\sum_1 = \sum_1^1 + \sum_1^2 + \sum_1^3 + \sum_1^4,$$

where

$$\begin{aligned} \sum_1^1 &= \sum_{y \in P_k} [(d_\Gamma(a).d_\Gamma(y))d_\Gamma(a, y) - (d_{\Gamma'}(a).d_{\Gamma'}(y))d_{\Gamma'}(a, y)] \\ &\quad + \sum_{y \in P_k} [(d_\Gamma(b).d_\Gamma(y))d_\Gamma(b, y) - (d_{\Gamma'}(b).d_{\Gamma'}(y))d_{\Gamma'}(b, y)] \\ &= (q - 1) \sum_{i=1}^k d_\Gamma(b_i) [d_\Gamma(a, b_i) - d_{\Gamma'}(a, b_i)]. \end{aligned}$$

With $d_\Gamma(a, b_i) = d_{\Gamma'}(b, b_i) + 1$, we have

$$\sum_1^1 = (q - 1) \sum_{i=1}^k d_\Gamma(b_i).$$

Let $\sum_{i=1}^k d_\Gamma(b_i) = \alpha$ and $\sum_{i=1}^l d_\Gamma(a_i) = \eta$, it follows that $\sum_1^1 = (q - 1)\alpha > 0$, since $q \geq 2$.

Now,

$$\begin{aligned} \sum_1^2 &= \sum_{y \in P_l} [(d_\Gamma(a).d_\Gamma(y))d_\Gamma(a, y) - (d_{\Gamma'}(a).d_{\Gamma'}(y))d_{\Gamma'}(a, y)] \\ &\quad + \sum_{y \in P_l} [(d_\Gamma(b).d_\Gamma(y))d_\Gamma(b, y) - (d_{\Gamma'}(b).d_{\Gamma'}(y))d_{\Gamma'}(b, y)] \\ &= \sum_{i=1}^l \{d_\Gamma(b, a_i) [(1 - q)d_\Gamma(a_i)] + d_\Gamma(a, a_i) [(q - 1)d_\Gamma(a_i)]\}. \end{aligned}$$

With $d_\Gamma(a, a_i) = d_{\Gamma'}(b, a_i) - 1$, we have $\sum_1^2 = (1 - q) \sum_{i=1}^l d_\Gamma(a_i) = (1 - q)\eta < 0$, since $q \geq 2$. Again

$$\begin{aligned} \sum_1^3 &= \sum_{y \in V(\mathbb{G})} [(d_\Gamma(a).d_\Gamma(y))d_\Gamma(a, y) - (d_{\Gamma'}(a).d_{\Gamma'}(y))d_{\Gamma'}(a, y)] \\ &\quad + \sum_{y \in V(\mathbb{G})} [(d_\Gamma(b).d_\Gamma(y))d_\Gamma(b, y) - (d_{\Gamma'}(b).d_{\Gamma'}(y))d_{\Gamma'}(b, y)] \\ &= \sum_{y \in V(\mathbb{G})} [t.d_\Gamma(y)d_\Gamma(b, y) - d_\Gamma(y)[t + q - 1][d_\Gamma(b, y) - 1]] \\ &\quad + \sum_{y \in V(\mathbb{G})} [(q + 1)d_\Gamma(y)d_\Gamma(a, y) - 2d_\Gamma(y)[d_\Gamma(a, y) + 1]]. \end{aligned}$$

As $d_\Gamma(a, y) = d_\Gamma(b, y) - 1$, and let $\sum_{y \in V(\mathbb{G})} d_\Gamma(y) = \pi$, we have

$$\sum_1^3 = t \sum_{y \in V(\mathbb{G})} d_\Gamma(y) = t\pi.$$

Lastly,

$$\begin{aligned} \sum_1^4 &= \sum_{x \in V(\mathbb{G}_1)} [(d_\Gamma(a).d_\Gamma(x))d_\Gamma(a, x) - (d_{\Gamma'}(a).d_{\Gamma'}(x))d_{\Gamma'}(a, x)] \\ &+ \sum_{x \in V(\mathbb{G}_1)} [(d_\Gamma(b).d_\Gamma(x))d_\Gamma(b, x) - (d_{\Gamma'}(b).d_{\Gamma'}(x))d_{\Gamma'}(b, x)]. \end{aligned}$$

With $d_{\Gamma'}(b, x) = d_\Gamma(b, x) + 1$, and let $\sum_{x \in V(\mathbb{G}_1)} d_\Gamma(x) = \varphi$, we have

$$\sum_1^4 = (q - 1) \sum_{x \in V(\mathbb{G}_1)} d_\Gamma(x) = (q - 1)\varphi.$$

Thus,

$$\sum_1 = \sum_1^1 + \sum_1^2 + \sum_1^3 + \sum_1^4 = (q - 1)[\alpha - \eta + \varphi] + t\pi > 0, \quad \text{as } \alpha > \eta.$$

Now, $\sum_2 = (q + 1)t(1) - 2(t + q - 1)(1) = (q - 1)(t - 2) > 0$, because $t \geq 2$. Also,

$$\begin{aligned} \sum_3 &= \sum_{\substack{x \in V(\mathbb{G}_1) \cup V(P_1) \setminus \{b\} \\ y \in V(\mathbb{G})}} [(d_\Gamma(x).d_\Gamma(y))d_\Gamma(x, y) - (d_{\Gamma'}(x).d_{\Gamma'}(y))d_{\Gamma'}(x, y)] \\ &= \sum_{y \in V(\mathbb{G})} d_\Gamma(y) \left[\sum_{i=1}^k d_\Gamma(b_i) - \sum_{i=1}^l d_\Gamma(a_i) + \sum_{x \in V(\mathbb{G}_1)} d_\Gamma(x) \right] \\ &= \pi[\alpha - \eta + \varphi] > 0. \end{aligned}$$

Thus, we obtain $Gut(\Gamma) > Gut(\Gamma')$. □

2.3. θ -transformation

To define θ -transformation, consider a nontrivial tree(bipartite graph) Γ . Let us take $ab \in E(\Gamma)$ a cut edge such that $d_\Gamma(b) = t (t \geq 2)$. Furthermore, let us consider a star S_{k+2} with central vertex r . The graph \mathbb{G} can be obtained by merging a vertex a in $V(\Gamma)$ with a pendant vertex of S_{k+2} . To perform this operation, we delete all edges rz and add new edges bz where z is a neighbor of r in S_{k+2} , except for a . The resulting graph is referred to as \mathbb{G}' , and this operation is known as a θ -transformation (refer to Figure 2.3).

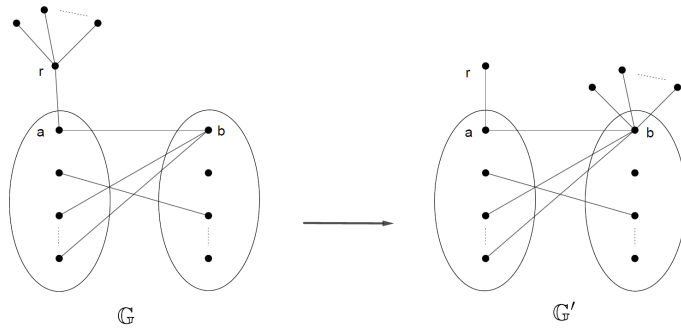


Figure 3. θ -transformation

Theorem 3. Let \mathbb{G}' be a connected graph obtained from \mathbb{G} by θ -transformation (see Figure 2.3). Then

$$Gut(\mathbb{G}) > Gut(\mathbb{G}').$$

Proof. To proof the inequality, one can see that its enough to compute

$$Gut(\mathbb{G}) - Gut(\mathbb{G}') = \sum_1 + \sum_2 + \sum_3,$$

where

$$\begin{aligned} \sum_1 &= \sum_{\substack{x \in \{r,b\} \\ y \in V(\mathbb{G}) \setminus \{r,b\}}} [(d_{\mathbb{G}}(x).d_{\mathbb{G}}(y))d_{\mathbb{G}}(x,y) - (d_{\mathbb{G}'}(x).d_{\mathbb{G}'}(y))d_{\mathbb{G}'}(x,y)] \\ \sum_2 &= (d_{\mathbb{G}}(r).d_{\mathbb{G}}(b))d_{\mathbb{G}}(r,b) - (d_{\mathbb{G}'}(r).d_{\mathbb{G}'}(b))d_{\mathbb{G}'}(r,b) \quad \text{and} \\ \sum_3 &= \sum_{\substack{z \in V(\Gamma) \setminus \{b\} \\ y \in N(r) \setminus \{a\}}} [(d_{\mathbb{G}}(z).d_{\mathbb{G}}(y))d_{\mathbb{G}}(z,y) - (d_{\mathbb{G}'}(z).d_{\mathbb{G}'}(y))d_{\mathbb{G}'}(z,y)], \end{aligned}$$

with $\sum_1 = \sum_1^1 + \sum_1^2$, where

$$\begin{aligned} \sum_1^1 &= \sum_{y \in V(\mathbb{G}) \setminus \{r,b\}} (d_{\mathbb{G}}(y).d_{\mathbb{G}}(r))d_{\mathbb{G}}(y,r) - \sum_{y \in V(\mathbb{G}) \setminus \{r,b\}} (d_{\mathbb{G}'}(y).d_{\mathbb{G}'}(r))d_{\mathbb{G}'}(y,r) \\ \sum_1^2 &= \sum_{y \in V(\mathbb{G}) \setminus \{r,b\}} (d_{\mathbb{G}}(y).d_{\mathbb{G}}(b))d_{\mathbb{G}}(y,b) - \sum_{y \in V(\mathbb{G}) \setminus \{r,b\}} (d_{\mathbb{G}'}(y).d_{\mathbb{G}'}(b))d_{\mathbb{G}'}(y,b). \end{aligned}$$

Now, we solve above entities independently.

$$\begin{aligned} \sum_1^1 &= \sum_{z \in V(\Gamma) \setminus \{b\}} (d_{\mathbb{G}}(z).d_{\mathbb{G}}(r))d_{\mathbb{G}}(z,r) - \sum_{y \in V(\mathbb{G}) \setminus \{r,b\}} (d_{\mathbb{G}'}(y).d_{\mathbb{G}'}(r))d_{\mathbb{G}'}(y,r) \\ &= \sum_{z \in V(\Gamma) \setminus \{b\}} [(d_{\mathbb{G}}(z).d_{\mathbb{G}}(r))d_{\mathbb{G}}(z,r) - (d_{\mathbb{G}'}(z).d_{\mathbb{G}'}(r))d_{\mathbb{G}'}(z,r)] \\ &\quad + \sum_{z \in V(S_{k+1}) \setminus \{r\}} [(d_{\mathbb{G}}(z).d_{\mathbb{G}}(r))d_{\mathbb{G}}(z,r) - (d_{\mathbb{G}'}(z).d_{\mathbb{G}'}(r))d_{\mathbb{G}'}(z,r)]. \end{aligned}$$

Since $d_{\mathbb{G}}(r) = k + 1$ and $d_{\mathbb{G}'}(z, r) = d_{\mathbb{G}}(z, r)$, so

$$\sum_1 = \sum_{z \in V(\Gamma) \setminus \{b\}} kd_{\mathbb{G}}(z)d_{\mathbb{G}}(z, r) + k(k - 2).$$

Now

$$\begin{aligned} \sum_1^2 &= \sum_{z \in V(\Gamma) \setminus \{b\}} [(d_{\mathbb{G}}(z).d_{\mathbb{G}}(b))d_{\mathbb{G}}(z, b) - (d_{\mathbb{G}'}(z).d_{\mathbb{G}'}(b))d_{\mathbb{G}'}(z, b)] \\ &+ \sum_{z \in V(S_{k+1}) \setminus \{r\}} [(d_{\mathbb{G}}(z).d_{\mathbb{G}}(b))d_{\mathbb{G}}(z, b) - (d_{\mathbb{G}'}(z).d_{\mathbb{G}'}(b))d_{\mathbb{G}'}(z, b)]. \end{aligned}$$

Since $d_{\mathbb{G}'}(b) = d_{\mathbb{G}}(b) + k = t + k$ and $d_{\mathbb{G}'}(z, b) = d_{\mathbb{G}}(z, b)$, so

$$\sum_1^2 = 2kt - k^2 - \sum_{z \in V(\Gamma) \setminus \{b\}} kd_{\mathbb{G}}(z)d_{\mathbb{G}}(z, b).$$

Thus $\sum_1 = \sum_1^1 + \sum_1^2 = 2k(t - 1) + \sum_{z \in V(\Gamma) \setminus \{b\}} 2kd_{\mathbb{G}}(z).$

Furthermore,

$$\begin{aligned} \sum_2 &= (d_{\mathbb{G}}(r).d_{\mathbb{G}}(b))d_{\mathbb{G}}(r, b) - (d_{\mathbb{G}'}(r).d_{\mathbb{G}'}(b))d_{\mathbb{G}'}(r, b) \\ &= 2(k + 1)t - 2(t + k) = 2k(t - 1). \end{aligned}$$

Now

$$\begin{aligned} \sum_3 &= \sum_{\substack{z \in V(\Gamma) \setminus \{b\} \\ y \in N(r) \setminus \{a\}}} [(d_{\mathbb{G}}(z).d_{\mathbb{G}}(y))d_{\mathbb{G}}(z, y) - (d_{\mathbb{G}'}(z).d_{\mathbb{G}'}(y))d_{\mathbb{G}'}(z, y)] \\ &= \sum_{z \in V(\Gamma) \setminus \{b\}} kd_{\mathbb{G}}(z)[d_{\mathbb{G}}(z, a) - d_{\mathbb{G}}(z, b) + 1] = \sum_{z \in V(\Gamma) \setminus \{b\}} 2kd_{\mathbb{G}}(z). \end{aligned}$$

Hence $Gut(\mathbb{G}) - Gut(\mathbb{G}') = \sum_1 + \sum_2 + \sum_3 = 4k(t - 1) + \sum_{z \in V(\Gamma) \setminus \{b\}} 4kd_{\mathbb{G}}(z) > 0$, since $t > 1$. \square

2.4. γ -transformation

The γ -transformation is defined as follows: Consider a nontrivial tree Γ . Then $\mathbb{G} = \mathbb{G}_{k,l}$ is acquired by merging $a_0 \in V(\Gamma)$ with the vertex a_0 and b_0 of paths $a_0a_1a_2 \dots a_k$, $b_0b_1b_2 \dots b_l$ respectively. The new graph is obtained graph as: $\mathbb{G}' = \mathbb{G}_{k+1,l-1} = \mathbb{G}_{k,l} + a_kb_l - b_{l-1}b_l$. (Figure 2.4)

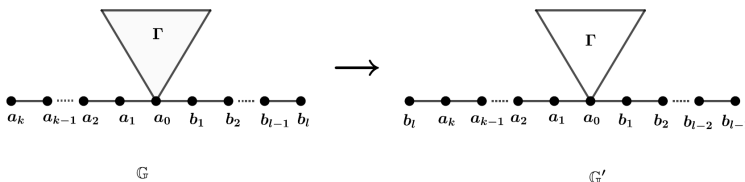


Figure 4. γ -transformation

Theorem 4. Let \mathbb{G}' be a connected graph obtained from \mathbb{G} by γ -transformation (see Figure 2.4). Then

$$Gut(\mathbb{G}) < Gut(\mathbb{G}').$$

Proof. Let $A_0 = \{a_k, b_{l-1}, b_l\}$ and $B_0 = V(\mathbb{G}_{k,l}) \setminus A_0$.

To proof the inequality, one can see that its enough to compute $Gut(\mathbb{G}) - Gut(\mathbb{G}') = \sum_1 + \sum_2$, where

$$\begin{aligned} \sum_1 &= \sum_{x \in B_0} [(d_{\mathbb{G}}(x).d_{\mathbb{G}}(a_k))d_{\mathbb{G}}(x, a_k) - (d_{\mathbb{G}'}(x).d_{\mathbb{G}'}(a_k))d_{\mathbb{G}'}(x, a_k)] \\ &\quad + \sum_{x \in B_0} [(d_{\mathbb{G}}(x).d_{\mathbb{G}}(b_{l-1}))d_{\mathbb{G}}(x, b_{l-1}) - (d_{\mathbb{G}'}(x).d_{\mathbb{G}'}(b_{l-1}))d_{\mathbb{G}'}(x, b_{l-1})] \\ &\quad + \sum_{x \in B_0} [(d_{\mathbb{G}}(x).d_{\mathbb{G}}(b_l))d_{\mathbb{G}}(x, b_l) - (d_{\mathbb{G}'}(x).d_{\mathbb{G}'}(b_l))d_{\mathbb{G}'}(x, b_l)]. \end{aligned}$$

Since $d_{\mathbb{G}'}(x, a_k) = d_{\mathbb{G}}(x, a_k)$, $d_{\mathbb{G}'}(x, b_{l-1}) = d_{\mathbb{G}}(x, b_{l-1})$ and $d_{\mathbb{G}'}(x, b_l) = d_{\mathbb{G}}(x, a_k) + 1$, $d_{\mathbb{G}}(x, b_l) = d_{\mathbb{G}}(x, b_{l-1}) + 1$, hence we have,

$$\sum_1 = \sum_{x \in B_0} 2d_{\mathbb{G}}(x)[(d_{\mathbb{G}}(x, b_{l-1}) - d_{\mathbb{G}}(x, a_k))].$$

Since $k \geq l$, so $\sum_{x \in B_0} (d_{\mathbb{G}}(x, b_{l-1}) < \sum_{x \in B_0} d_{\mathbb{G}}(x, a_k)$, implies that $\sum_1 < 0$. Now, we consider

$$\begin{aligned} \sum_2 &= \sum_{x,y \in A_0} [(d_{\mathbb{G}}(x).d_{\mathbb{G}}(y))d_{\mathbb{G}}(x, y) - (d_{\mathbb{G}'}(x).d_{\mathbb{G}'}(y))d_{\mathbb{G}'}(x, y)] \\ &= [(d_{\mathbb{G}}(b_{l-1}).d_{\mathbb{G}}(a_k))d_{\mathbb{G}}(b_{l-1}, a_k) - (d_{\mathbb{G}'}(b_{l-1}).d_{\mathbb{G}'}(a_k))d_{\mathbb{G}'}(b_{l-1}, a_k)] \\ &\quad + [(d_{\mathbb{G}}(b_l).d_{\mathbb{G}}(b_{l-1}))d_{\mathbb{G}}(b_l, b_{l-1}) - (d_{\mathbb{G}'}(b_l).d_{\mathbb{G}'}(b_{l-1}))d_{\mathbb{G}'}(b_l, b_{l-1})] \\ &\quad + [(d_{\mathbb{G}}(a_k).d_{\mathbb{G}}(b_l))d_{\mathbb{G}}(a_k, b_l) - (d_{\mathbb{G}'}(a_k).d_{\mathbb{G}'}(b_l))d_{\mathbb{G}'}(a_k, b_l)]. \end{aligned}$$

Since $d_{\mathbb{G}}(b_l, a_k) = d_{\mathbb{G}'}(b_{l-1}, b_l) = k + l$, and $d_{\mathbb{G}'}(b_{l-1}, a_k) = d_{\mathbb{G}}(b_{l-1}, a_k)$, thus we have

$$\sum_2 = k + l - 2 - k - l + 2 = 0,$$

which implies that $Gut(\mathbb{G}) - Gut(\mathbb{G}') = \sum_1 + \sum_2 < 0$, and that complete the proof. □

3. Results and Discussions

Let us consider the class of trees Γ_n^a of order n with a leaves. If $a = 1$ or $a = n - 1$, we have unique tree. Thus we will take only $3 \leq a \leq n - 2$. Let us denote the class of trees Γ_n^d of order n with a given diameter d . In this section, we will give the extremal results for these two classes of trees. A tree Γ is called a spider if it has at most one

vertex u with d_u is greater than 2 which is known as the hub of the spider and its legs are made by paths from its leaves to the hub. Now, we will denote $\mathbb{S}(l_1, l_2, \dots, l_a)$ the n -vertex spider along P_1, P_2, \dots, P_a legs such that every leg P_i is of length l_i for all $i = 1, 2, \dots, a$ and $\sum_{i=1}^a l_i = n - 1$. A spider $\mathbb{S}(l_1, l_2, \dots, l_a)$ is known to be a balanced spider if $|l_i - l_j| \leq 1$ for all $1 \leq i, j \leq a$. It is known that any balanced spider of order n is isomorphic to $\mathbb{S}\left(\underbrace{\lfloor \frac{n-1}{a} \rfloor, \dots, \lfloor \frac{n-1}{a} \rfloor}_{n-t}, \underbrace{\lceil \frac{n-1}{a} \rceil, \dots, \lceil \frac{n-1}{a} \rceil}_t\right)$ such that $n - 1 \equiv t \pmod{a}$. Now, we will give our results related with the class Γ_n^a of order n with a given number of leaves a .

Theorem 5. *The minimum value of Gutman index in the class Γ_n^a is attained by the unique balanced spider tree $\mathbb{S}\left(\underbrace{\lfloor \frac{n-1}{a} \rfloor, \dots, \lfloor \frac{n-1}{a} \rfloor}_{n-t}, \underbrace{\lceil \frac{n-1}{a} \rceil, \dots, \lceil \frac{n-1}{a} \rceil}_t\right)$ such that $n-1 \equiv t \pmod{a}$*

Proof. Let Γ be the tree in the class Γ_n^a such that $Gut(\Gamma)$ is the smallest. It is sufficient to prove that Γ is a balanced spider. On contrary, supposed that Γ is not a spider. Then by Theorem 2, we can get a tree Γ' by using β transformation on Γ such that $Gut(\Gamma') < Gut(\Gamma)$. It is contradiction to our supposition that Γ attains the smallest value of Gutman index. In order to complete the proof, we need to show that $\Gamma \cong \mathbb{S}\left(\underbrace{\lfloor \frac{n-1}{a} \rfloor, \dots, \lfloor \frac{n-1}{a} \rfloor}_{n-t}, \underbrace{\lceil \frac{n-1}{a} \rceil, \dots, \lceil \frac{n-1}{a} \rceil}_t\right)$ is a balanced spider for $n - 1 \equiv t \pmod{a}$. Again suppose that $\Gamma = \mathbb{S}(l_1, l_2, \dots, l_a)$. Now if Γ is not a balanced, then it must have at least two P_i, P_j legs of lengths l_i, l_j such that $|l_i - l_j| \geq 2$. Let us consider $P_i = a_1 a_2, \dots, a_i$ and $P_j = b_1 b_2, \dots, b_j$ for $j < i$, be the two such legs of Γ . then we will obtain $\Gamma'' \neq \Gamma$ by deleting $b_{j-1} b_j$ from P_j and adding $b_j a_i$ in P_i . Now by applying Theorem 4, we will get $Gut(\Gamma'') < Gut(\Gamma)$, which is the contradiction, hence the proof finished. \square

Let $P_{d+1} = x_0 x_1 \dots x_d$ be the d -length path. Then $\Gamma(y_1, y_2, \dots, y_{d-1})$ be the tree obtained from P_{d+1} by connecting y_i pendant vertices to each of x_i , for all $1 \leq i \leq d-1$ and $n = d + 1 + \sum_{i=1}^{d-1} y_i$. Let us consider such tree $\Gamma(0, 0, \dots, 0, y_{\lfloor \frac{d}{2} \rfloor}, 0, \dots, 0)$. Let us denote the class of all tree of order n with diameter d by Γ_n^d . We will characterize in the following result the tree which obtained the smallest value of Gutman index in Γ_n^d .

Theorem 6. *The smallest value of Gutman index in the class Γ_n^d is attained by the tree $\Gamma(0, 0, \dots, 0, y_{\lfloor \frac{d}{2} \rfloor}, 0, \dots, 0)$.*

Proof. Let Γ be the tree in the class Γ_n^d such that $Gut(\Gamma)$ is the smallest and

$$\Gamma \neq \Gamma(0, 0, \dots, 0, y_{\lfloor \frac{d}{2} \rfloor}, 0, \dots, 0).$$

Either multiple vertices have degree greater than 2, or there is only one vertex x_2 with $d_\Gamma(x_2) > 2$ s. t. it has a path of length greater than two length one attached to it. Let $P = x_0x_1 \cdots x_d$ be the longest path attached to x_2 . Then by α -transformation on such vertices, we can get Γ' s. t. $\Gamma' \neq \Gamma$. Now by Theorem 1, we get the inequality $Gut(\Gamma') < Gut(\Gamma)$, which is the contradiction to the minimality of $Gut(\Gamma)$, similarly, other case can be proved, which complete the proof. \square

In graph theory, a matching in a graph G is a set of edges that do not have a set of common vertices. In other words, a matching is a graph where each node has either zero or one edge incident to it. The maximum cardinality of such set of edges is called matching number of G and denoted by $\nu(G)$. A dominating set for a graph G is a subset D of the vertices such that every vertex not in D is adjacent to at least one member of D . The domination number $\omega(G)$ is the number of vertices in a smallest dominating set for G . We have the following relation between matching number and domination number of a graph G .

Theorem 7 ([13]). *If G is any connected graph, then $\omega(G) \leq \nu(G)$*

Lemma 1 ([4]). *Let T be an n -vertex tree. Then $Gut(S_n) \leq Gut(T) \leq Gut(P_n)$.*

Let us consider the class of trees Γ_n^ω of order n with domination number ω . Now we will give characterization of minimal trees with domination number ω in this class which achieve the minimum values for the Gutman index.

Theorem 8. *If Γ has the smallest value of Gutman index in the class Γ_n^ω , then $\omega(\Gamma) = \nu(\Gamma)$*

Proof. Let Γ has domination number ω and matching number ν . then by theorem 8, we have $\omega(\Gamma) \leq \nu(\Gamma)$. Thus it is enough to prove that $\omega(\Gamma) \geq \nu(\Gamma)$. On contrary, supposed that $\omega(\Gamma) < \nu(\Gamma)$ and a set of cardinality ω which is dominating set as well denoted by $A = \{a_1, a_2, \dots, a_\omega\}$ is a dominating set of cardinality ω . Thus, we have $a_1a'_1, a_2a'_2, \dots, a_\omega a'_\omega$ independent edges. Let us consider the set $M' = \{a_i a'_i : i = 1, 2, \dots, \omega\}$, then M' must be subset of any maximal matching M , because $\omega(\Gamma) < \nu(\Gamma)$. Thus there is at least one edge b_1b_2 , which is not connected with each of the edges $a_i a'_i$ for all $i = 1, 2, \dots, \omega$. By the similar argument given in [20], we can always find a matching M , such that Γ will have $\omega + 1$ edges $a_1a'_1, a_2a'_2, \dots, a_\omega a'_\omega, b_1b_2$. Now, if there is unique vertex of A whihc dominate the b_1, b_2 , then we have a triangle 3 in Γ which is not possible as Γ is a tree.

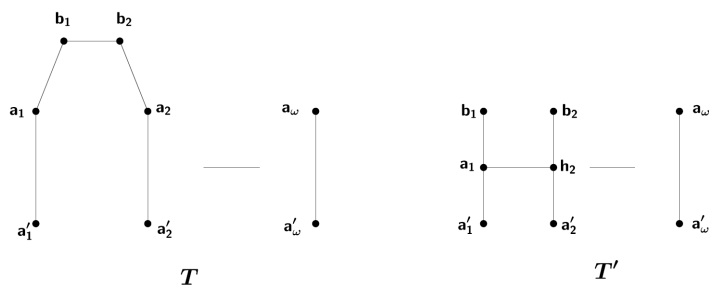


Figure 5. The structure of Γ and Γ' trees

Thus, two different vertices of A must dominate both vertices b_1 and b_2 . Let us suppose that b_j is dominated by a vertex a_j , where $j = 1, 2$ as shown in Fig. (5). If we apply α -transformation on a_1b_1 and a_2b_2 of the tree Γ , we will get Γ' as shown in Figure 5. Then by applying Theorem 1, we get $Gut(\Gamma') < Gut(\Gamma)$, which is the contradiction to the minimality of $Gut(\Gamma)$, which complete the proof. \square

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